TITLE: Large Eddy Simulations of Supercritical Multicomponent Mixing Layers

LARGE EDDY SIMULATIONS OF SUPERCRITICAL MULTICOMPONENT MIXING LAYERS

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SUMMARY/OVERVIEW:

The objective of this study is the fundamental understanding of fuel disintegration and mixing in a supercritical environment (relative to the fuel) in order to determine parameter regimes advantageous to mixing. The approach is based on developing a model of a supercritical, turbulent jet mixing with surrounding fluid. The method is one that combines the modeling of supercritical fluids with a systematic development based on the Large Eddy Simulation (LES) approach. This systematic development includes a consistent protocol based upon Direct Numerical Simulations (DNS) for developing a Subgrid Scale Model (SGS) appropriate to supercritical fluids, rather than choosing in an ad hoc manner an existing SGS model developed under assumptions inconsistent with supercritical fluid behavior. This SGS model will be used in the LES of a supercritical turbulent jet.

TECHNICAL DISCUSSION

The first step in this effort consisted in the development of a DNS and associated code for a supercritical shear layer. The shear layer is chosen as the simplest configuration from which one may obtain results that will establish, through DNS, a framework for understanding mixing of supercritical fluids at small scales. Because the turbulent behavior at the Kolmogorov scales is universal (i.e. geometric-configuration independent), once this behavior is determined (e.g. in a shear layer geometric configuration), it can be utilized to model a variety of geometric configurations (for the same fluids) having the same physics. Since the interest of AFOSR is in hydrocarbons, the chosen shear layer is that of heptane (lower stream) in nitrogen. Having conducted preliminary investigations in which the layer did not reach transition (Miller et al., 2001), and having analyzed the causes for the lack of transition (Okong'o and Bellan, 2000a), the activities were further focused on obtaining one or several transitional states and analyzing their behavior. To this end, there were several areas of emphasis:

(i) The real-gas boundary conditions of Okong'o and Bellan, 2000b (OB00jcp) were utilized in the DNS code and two simulations were conducted differing only by the value of the initial Reynolds number; the wavelength of the initial forcing was the typical one from the incompressible stability analysis. The results were documented in Okong'o and Bellan, 2000c (OB00jfm).

The transitional state was identified by global manifestations such as rapid and sustained momentum thickness growth, high rate of positive spanwise vorticity evolution, increased enstrophy, large product thickness, and large momentum thickness based Reynolds number. Analysis of the vorticity and vorticity magnitude budgets at transition highlighted the dominance of the stretching and tilting effect in the production of spanwise vorticity, and of the viscous contribution in the vorticity magnitude, although at some crosstream locations stretching and tilting exceeded viscous effects.

Visualizations of the spanwise vorticity at the transitional state revealed considerable local positive vorticity both in the braid and between the braid planes. Furthermore, visualizations of the magnitude of the density gradient displayed concentrated regions of high values exhibiting a convoluted and distorted appearance; these regions may be optically identifiable owing to the change in the index of refraction. Given the commonality of distinctive optical features between temporal and spatial shear layers, the observation of such regions in supercritical jet experiments provided encouragement that the essence of the situation has been captured. Analysis of the fluid composition in these regions of high density gradient magnitude revealed that the predominant species is that in the lower, entrained stream with small amounts of the entraining fluid transported and dissolved into it. Moreover, considerations based on the value of the mass diffusion factor identified these regions to contain a highly non-ideal mixture, implying mixing difficulties at the molecular level resulting from the thermodynamic properties of the mixture. Visualizations of the compression factor displayed large departures from perfect gas behavior in the lower heptane stream as well as in the layer.

The issue of the thermodynamic state of the mixture at transition was also explored through examination of departures from the critical locus both in the braid and between braid planes. The fluid was supercritical everywhere, as the temperature was always larger than that of the local critical point. However, the pressure was above the local critical point outside and below the local critical point inside the vortices, with the critical locus mapping the coherent vortices. The considerable reduction in the difference between the local values of the pressures and critical pressure inside the vortices was due to the change in fluid composition.

To investigate the primary mechanisms responsible for dissipation both during the evolution of the layer and at transition, the irreversible entropy production was calculated and analyzed. The three contributions to the dissipation arising from viscous stresses, species fluxes and heat fluxes were calculated and compared. Volume averages as well as RMS were computed at time stations after the second pairing, but prior to transition, and at transition. Moreover, by filtering the DNS solution and calculating the difference between the filtered and unfiltered variables, the contribution of the small scales (SGS) was evaluated. The overwhelming SGS contribution both to the average and the RMS is due to viscous effects, and the SGS activity is also dominated by viscous effects.

Since the transitional state was dominated by viscous effects, one could argue that the above conclusions are universal, i.e. independent of the species and only governed by the supercritical state. Such an argument may be in error since some of the important aspects of the transitional state, such as the fluid composition in the high magnitude density regions may be a result of the mixture thermodynamics. Ascertaining the species independent aspects of supercritical mixing layer behavior will constitute one of our future priorities.

Assumed PDF modeling, of particular interest for reacting flow representations, was shown to have only limited potential. Neither the beta-density nor the Gaussian PDF, both constructed using the DNS calculated moments, predicted reliably the mixing process or the transitional state, respectively. The same result was found at the subgrid scale. Moreover, the temperature and partial density PDFs were well (negatively) correlated, indicating that the possible modeling of the reaction rate, which is a joint temperature-species PDF, by the product of the marginal PDFs holds poor prospects. This good correlation was obtained both for the DNS scale PDF and the SGS scale PDF (the filtered density function of Pope, 1991). Finally, it should be mentioned that the conclusions regarding the PDF representation are the result of studying only two realizations. It was realized that additional work is necessary to obtain more definitive conclusions.

(ii) The investigation described in (i) indicated the need for additional realizations of transitional states. However, each DNS simulation is very computationally intensive, and thus a good strategy was deemed necessary to minimize computational costs. Therefore, a linear inviscid stability analysis for real gas was conducted with the goal of finding other forcing wavelengths that perhaps promote quicker transition. The results of the stability analysis and the ensuing simulations were documented in Okong'o and Bellan, 2001. Two-dimensional (2D) stability results showed that the unstable growth rates for the compressible flow are smaller at all wavenumbers than the equivalent growth rates found from an incompressible analysis; also, the most unstable wavelengths occurred at smaller wavenumbers with increasing density stratification. 2D mixing layer simulations showed that at the same initial mean flow conditions the solution is virtually independent of the excitation wavelength. This observation raised the alluring prospect of finding the shortest streamwise compressible unstable wavelength at which rollup and pairing could be obtained in three-dimensional (3D) simulations; for such a wavelength, the size of the domain could be reduced (since it is four times the perturbation wavelength) leading to a reduced number of grid points for the same resolution. However, in contrast with the 2D problem where for each wavelength there is a single eigenvalue (i.e. propagation speed), in 3D it was found that additional to the wavelength of the perturbation, the angle of the wave direction in the streamwise-spanwise plane must be specified as well. To minimize the wavelength of the spanwise perturbation, it was shown that one must maximize the angle representing the direction of the perturbation. For the purpose of applications to 3D flow simulations, this implies that shorter wavelengths in the streamwise direction are counter balanced by the need to use a longer wavelength in the spanwise direction. Therefore, to avoid enlarging the spanwise domain size, the heuristic approach of using non-eigenfunction perturbations was adopted and simulations conducted for five shear layer were compared; for each of these simulations the streamwise domain size was four times the perturbation wavelength and the calculation was initiated with four vortices leading after two pairings to an ultimate vortex. Among these five simulations, two layers (differing by the value of the initial Reynolds number) were excited with the incompressible most unstable wavelength. The third and fourth layers (differing by the value of the initial Reynolds number) were excited with the shortest compressible unstable wavelength from the 2D stability analysis and the same amplitudes as the first two layers. The fifth layer was excited with the shortest compressible unstable wavelength from the two-dimensional stability analysis and a larger amplitude of the 3D excitation. Only three of these five layers achieved transition, and the expectation of reduced CPU time for the layer perturbed with the shortest compressible unstable wavelength did not materialize. Global evolution and contour plots showed that the inability of transition achievement by two of the layers perturbed with the shortest compressible unstable wavelength is due either to the inability of the formed small scales to produce substantial vorticity or to the early formation of small scales and vorticity production which destroy the coherence of the ultimate vortex preventing its growth and initiating its decay.

The results showed that transitional states with the same momentum thickness based Reynolds number can be achieved by perturbing with a variety of unstable wavelengths, and that they require similar CPU time. Simulations performed with a shorter wavelength perturbation require larger initial Reynolds numbers to reach a transitional state. Transitional states obtained with different perturbation wavelengths had different global and detailed characteristics, and therefore such simulations were recommended for enlarging the database necessary to extract turbulence models utilizable in the mathematical description of turbulent spatial flows.

Further investigations are now devoted to enlarging the transitional states database by (1) considering other binary system species, particularly those for which contemporary experimental information is available (e.g. LOX/He), and (2) considering additional perturbation wavelengths to obtain transitional states with different characteristics.

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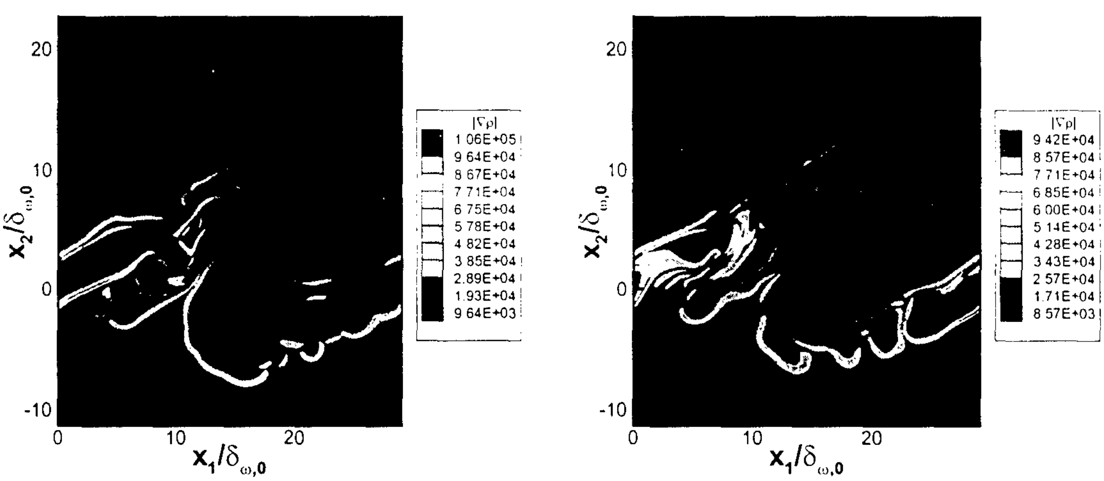

Figure 1 Density Gradient Magnitude at t*=135 (corresponding to the attainment of a transitional state), in the braid plane (left) and in the between-the-braid plane (right). The initial Reynolds number is 600, the initial Mach number is 0.4, and the freestream temperatures are 1000 K for the upper, nitrogen, stream and 600 K for the lower, heptane, stream.